Sensitivity analysis, parameter inversion, and design of experiments under uncertainty

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Consider a mathematical model that depends on random parameters

\[ y = f(x_1, x_2, \ldots, x_n) \]

Problem: assess the relative contribution of each input parameter to variance/uncertainty in \( f \)

Some reasons for doing this:

- Can lead to a better understanding of the model
- Can help in understanding the influence of uncertainties on predictions
- Can guide dimension reduction—fix inessential parameters at nominal values
- Can help in making parameter estimation more efficient—estimate only “important” parameters
Global sensitivity analysis (GSA): definitions

\[ y = f(x_1, x_2, \ldots, x_n) \]

Some global sensitivity indices:

- Variance based
  \[ S_i = \frac{\text{Var}\{E\{f|x_i\}\}}{\text{Var}\{f\}} \]

- Derivative based
  \[ \nu_i = \int \left( \frac{\partial f}{\partial x_i}(x) \right)^2 \pi(x) dx \]

Computing sensitivity indices requires repeated evaluations of \( f \)

For many years researchers considered GSA for \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), with \( x_i \) independent.


Example: $CO_2$ sequestration in geological formations

Expensive model, time/space dependent observables, correlations


- Physical process: non-isothermal, multiphase flow in porous media
- Governing equations: coupled, nonlinear, time-dependent system of PDEs
- Uncertainties in: porosity, absolute permeability, permeability of leaky well, injection rate, etc.
- A key observable: maximum $CO_2$ leakage ratio at the leaky well
- Global sensitivity analysis: understand relative contribution of model parameters to $CO_2$ leakage variability
Ocean general circulation model, Gulf of Mexico, Hurricane Ivan (2004)

- Governing equations: Navier–Stokes equations, transport equations for temperature, salinity
- Uncertainties in: subgrid scale, wind drag parameterization
- Key observables: sea surface temperature (SST), sea surface height (SSH), ...
- Global sensitivity analysis: understand relative contribution of model parameters to variability in SST, SSH, etc.
Example: stochastic genetic oscillator

Stochastic model, time-dependent observables, multiple scales

- Stochastic genetic oscillator
- Biochemical reaction network consisting of nine species and sixteen reactions
- Uncertainties in reaction rates
- Key quantities: concentration of proteins $A$ and $R$

Global sensitivity analysis: quantify relative contribution of random reaction rates to uncertainties in protein concentrations

Global sensitivity analysis (GSA): research directions

- Methods/theory for GSA with functional (time/space dependent) outputs*
- Methods/theory for GSA with stochastic time-dependent outputs
- Methods/theory for GSA with correlated variables
- Relations between derivative-based/variance-based indices for functional/stochastic quantities

Inverse problems and optimal design of experiments
Example: Diffusive transport of a contaminant with uncertain initial condition

- **Governing PDE** (forward model): advection-diffusion equation
- **Unknown/uncertain parameter**: initial concentration field
- **Inverse problem**: Use a vector $d$ of space/time sensor measurements of concentration to reconstruct the initial state
2D Model problem

- Forward problem: time dependent advection-diffusion

\[ u_t - \kappa \Delta u + \mathbf{v} \cdot \nabla u = 0 \quad \text{in } D \times [0, T] \]
\[ u(0, \mathbf{x}) = m \quad \text{in } D \]
\[ \kappa \nabla u \cdot \mathbf{n} = 0 \quad \text{on } \partial D \times [0, T] \]

- \( m \): unknown initial condition
- \( \mathbf{v} \): velocity field
Solution of the forward problem

$t = 0$

$t = 1$

$t = 2$

$t = 3$
The inverse problem: reconstruct initial condition

The inverse problem of finding the unknown initial state based on sensor data

\[
\min_m \frac{1}{2} \| \mathcal{B} u(m) - d \|^2 + \frac{\alpha}{2} \langle A m, m \rangle
\]

where

\[
\begin{align*}
 u_t - \kappa \Delta u + \mathbf{v} \cdot \nabla u &= 0 \quad \text{in } \mathcal{D} \times [0, T] \\
 u(0, x) &= m \quad \text{in } \mathcal{D} \\
 \kappa \nabla u \cdot \mathbf{n} &= 0 \quad \text{on } \partial \mathcal{D} \times [0, T]
\end{align*}
\]

- \( \mathcal{B} \): observation operator
- \( d = [d_1^T d_2^T \cdots d_n^T]^T, \quad d_i \in \mathbb{R}^{n_s}, n_s = \text{number of sensors} \)
- \( u \) linear in \( m, u = S m \implies \) linear parameter-to-observable map: \( \mathcal{F} = \mathcal{B} S \)
- Can rewrite the optimization problem as

\[
\min_m \mathcal{J}(m) := \frac{1}{2} \| \mathcal{F} m - d \|^2 + \frac{\alpha}{2} \langle A m, m \rangle
\]
Solving the inverse problem

- Derivative of $\mathcal{J}$

\[
D\mathcal{J}(m)(\tilde{m}) = \frac{d}{d\varepsilon}\mathcal{J}(m + \varepsilon\tilde{m}) \bigg|_{\varepsilon=0} = \langle \mathcal{F}^*(\mathcal{F}m - d) + \alpha Am, \tilde{m} \rangle
\]

- Action of $\mathcal{F}^*$

$\mathcal{F}^* y = p(\cdot, 0)$, where $p$ is solution of the adjoint equation

\[
-p_t - \nabla \cdot (p v) - \kappa \Delta p = -B^* y
\]

$p(T) = 0$

$(v p + \kappa \nabla p) \cdot n = 0$

- Optimality condition

\[
(\mathcal{F}^* \mathcal{F} + \alpha A)m = \mathcal{F}^* d \quad \text{discretize} \quad (F^*F + \alpha A)m = F^*d
\]

Solve the linear system using an iterative method, e.g. conjugate gradient
Solving the inverse problem: numerical results

Truth  Sensor sites  Reconstruction
Solving the inverse problem: numerical results

Truth  Sensor sites  Reconstruction
How to place sensors in an “optimal” way?

- Can formulate the optimal sensor placement problem as an optimal experimental design (OED) problem
- Can consider a statistical formulation of the inverse problem
- In addition to a reconstruction, we can also compute a statistical distribution of the parameters, conditioned on experimental data
- Find sensor locations so as to optimize the statistical quality of the reconstructed/inferred parameter
- In context of inverse problems a Bayesian formulation is natural
Bayesian inference: Bayes’ formula

\[ \pi_{\text{post}}(m|d) \propto \pi_{\text{like}}(d|m) \pi_{\text{prior}}(m) \]

- \( \pi_{\text{post}}(m|d) \): posterior pdf of \( m \)
- \( \pi_{\text{like}}(d|m) \): pdf of \( d \) given \( m \) (data likelihood)
- \( \pi_{\text{prior}}(m) \): prior pdf of \( m \)

pdf = probability density function

Rev. Thomas Bayes

Pierre-Simon Laplace

Bayes, T., An Essay towards Solving a Problem in the Doctrine of Chances. By the Late Rev. Mr. Bayes, FRS Communicated by Mr. Price, in a Letter to John Canton, AMFRS. Philosophical Transactions, 1763.

Laplace, P.S., Théorie analytique des probabilités. 1820.
Bayesian linear inverse problems

Assume linear parameter-to-observable map:
\[ d = Fm + \eta \]

and assume prior is Gaussian
\[ \pi_0(m) \propto \exp\left( -\frac{1}{2} m^T \Gamma_{\text{prior}}^{-1} m \right) \]

Then, the posterior pdf is
\[ \pi_{\text{post}}(m|d) \propto \exp \left\{ -\frac{1}{2} (m - m_{\text{MAP}})^T F^T \Gamma_{\text{noise}}^{-1} F + \Gamma_{\text{prior}}^{-1} \right\} (m - m_{\text{MAP}}) \]

\[ \Rightarrow \mu_{\text{post}} = \mathcal{N}(m_{\text{MAP}}, \Gamma_{\text{post}}) \]

\[ \Gamma_{\text{post}}^{-1} = \underbrace{F^T \Gamma_{\text{noise}}^{-1} F}_{H_{\text{misfit}}} + \Gamma_{\text{prior}}^{-1} \]

\[ m_{\text{MAP}} = \arg\min_m \frac{1}{2} \|Fm - d\|_{\Gamma_{\text{noise}}^{-1}}^2 + \frac{1}{2} \left\langle \Gamma_{\text{prior}}^{-1} m, m \right\rangle \]

An important problem structure:
\[ H_{\text{misfit}} \text{ is low rank, and } \Gamma_{\text{prior}}^{1/2} H_{\text{misfit}} \Gamma_{\text{prior}}^{1/2} \text{ is even more so ...} \]
Bayesian inversion of the initial condition for 2D advection-diffusion equation

- Posterior mean, and posterior variance
  - truth
  - posterior mean
  - posterior std deviation

- Posterior samples: \( \nu = \mathbf{m}_{\text{MAP}} + \mathbf{r}_{\text{post}}^{1/2} \mathbf{M}^{-1/2} \mathbf{n}, \quad \mathbf{n} \sim \mathcal{N}(0, \mathbf{I}) \)
The optimal experimental design problem

A grid of candidate locations for observation points

- **Experimental design**: locations of observation points / sensors
  
  $\text{design} := \{ x_1, \ldots, x_{N_s}, w_1, \ldots, w_{N_s} \}$

- **Bayesian inversion**: 
  
  data + likelihood, prior $\implies$ posterior distribution of inversion parameter

- **Optimal experimental design (OED)**: 
  
  Find sensor locations that result in minimized posterior uncertainty
Commonly used OED criteria

Bayesian A-optimal experimental design:

$$\min_{\mathbf{w} \in \mathcal{S}} \text{tr} \left[ \mathbf{\Gamma}_{\text{post}}(\mathbf{w}) \right] + \gamma P(\mathbf{w})$$ (1)

Bayesian D-optimal experimental design:

$$\min_{\mathbf{w} \in \mathcal{S}} - \frac{1}{2} \log \det(\mathbf{I} + \mathbf{\Gamma}_{\text{prior}}^{1/2} \mathbf{H}_{\text{misfit}}(\mathbf{w}) \mathbf{\Gamma}_{\text{prior}}^{1/2}) + \gamma P(\mathbf{w})$$ (2)

- Need trace/log-determinant of high-dimensional operators
- Need many applications of the forward operator \(\Rightarrow\) many PDE solves
- OED much harder for nonlinear inverse problems
- Ingredients of efficient OED methods: randomized matrix methods, use of problem structure, low-rank approximations, iterative solvers, gradient based optimization algorithms, adjoint based gradient/Hessian computation, sparsifying penalty methods, ...


A-optimal design: the variance field

Optimal

Sub-optimal
A-optimal design: the variance field

Optimal

Sub-optimal
A-optimal design: the variance field

Optimal

Sub-optimal
A. Alexanderian, N. Petra, G. Stadler, and O. Ghattas. A-optimal design of experiments for infinite-dimensional Bayesian linear inverse problems with regularized $\ell^0$-sparsification. SISC. 2014.
Summary and outlook

Global sensitivity analysis: Apportion uncertainty in the model output to different sources of uncertainty in the model input parameters

- Interesting directions: theory and efficient computational methods for global sensitivity analysis with high-dimensional/functional outputs, stochastic models, correlated random inputs

- Applications: multiphase flow through porous media, radio-active waste storage, biotransport in cancerous tumors, chemical kinetics, biochemistry, epidemiology, ...

- NCSU faculty collaborators: Pierre Gremaud, Ralph Smith
Optimal sensor placement for Bayesian linear inverse problems: find optimal placements of measurement point to minimize the uncertainty in reconstructed parameters

- Interesting research directions: scalable algorithms for A-optimal sensor placement for Bayesian inverse problems governed by PDEs (randomized methods in numerical linear algebra, low-rank approximations, optimization with exact penalty method, ...);
- Optimal sensor placement for Bayesian nonlinear inverse problems* (bi-level PDE-constrained optimization, adjoint based derivative computation, ...)
- Applications: porous medium flow, contaminant source identification, radiation detection in urban environments

NCSU faculty collaborators: Arvind Saibaba, Ralph Smith

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